

**International Focus Workshop on  
Quantum Simulations and Design  
27 to 29 September 2011**

The International Focus Workshop on Quantum Simulations and Design (QSD11) was held at the Max Planck Institute for the Physics of Complex Systems in Dresden (MPIPKS), Germany, from 27 to 29 September 2011. This conference was organized under the auspices of the MPIPKS and the Grant-in-Aid for Scientific Research on Innovative Areas “Materials Design through Computics: Complex Correlation and Nano-Equilibrium Dynamics”, MEXT, Japan.

The conference focused on the development of methods for first principles electronic structure calculations and their applications. The aim was to provide an opportunity for discussion on the progress in computational materials design and, in particular, the development of quantum simulations and quantum design. A second goal was to strengthen the exchange and cooperation between European researchers with Japanese partners.

Computational materials design is a computational approach for the development of new materials. The essential ingredient is the use of quantum simulations to design a material that meets a given specification of properties and functionality. For this to be successful, the simulation has to be very reliable and be applicable to systems of realistic size.

During the conference, new approaches were discussed including methods beyond the local density approximation of density functional theory, order- $N$  methods, methods dealing with excitations, reactions and finite temperatures, and the application of these methods to the design of novel materials, devices and systems.

The conference provided an international forum for experimental and theoretical researchers to exchange ideas. A total of 50 delegates from ten countries participated in the conference. There were 14 invited talks and 18 contributed oral presentations. Young researchers were given a platform to present their work in front of the experts, allowing invited (3) as well as contributed talks (7) for them. Ample time for discussion was given in two poster sessions with 18 contributions presented. Important highlights of the workshop were the talks of the invited speakers:

- Prof. Igor Abrikosov (Linköping University, Sweden)
- Prof. Hisazumi Akai (Osaka University, Japan)
- Prof. Gerrit Bauer (Delft University of Technology, Netherlands)
- Dr. Markus Eisenbach (Oak Ridge National Laboratory, USA)
- Prof. Olle Eriksson (Uppsala University, Sweden)
- Dr. Martin Gradhand (University of Bristol, UK)
- Prof. Koichiro Inomata (National Institute for Materials Science, Tsukuba) **(E)**
- Prof. Takao Kotani (Tottori University, Japan)
- Dr. Jan Minar (Ludwig-Maximilians-University, München, Germany)
- Prof. A. Oshiyama (University of Tokyo, Japan)
- Dr. Mark Stiles (NIST, USA)
- Prof. Shinji Tsuneyuki (University of Tokyo, Japan)
- Prof. Wulf Wulfhekel (Universität Karlsruhe (TH), Germany) **(E)**

The talks, mostly of colleagues active in the field of theory were complemented by contributions of two colleagues from experiment **(E)** who presented the state of the art in GMR- and TMR devices and spin-resolved STM.

Altogether the stimulating atmosphere of the workshop venue led to very lively and fruitful discussions. Following to the great and positive resonance among the participants it was agreed to organize a similar workshop in 2013.